

The non-linear elastic behavior and ideal shear strength of Al and Cu

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Abstract

We present recent *ab initio* calculations of the ideal shear strengths of aluminum and copper using pseudopotential density functional theory within the local density approximation. Structural relaxations orthogonal to the applied shear significantly reduce the values of ideal shear strength, resulting in strengths of 8–9% of the shear modulus for both Al and Cu. However, the geometry of the relaxations in Al and Cu is very different. To some degree, this can be explained using experimentally measured third-order elastic constants. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Given recent advances in theoretical methods and computing machinery, it has become possible to compute the low-temperature elastic behavior of elemental solids and ordered compounds with encouraging accuracy [1]. Since the linear elastic constants of almost all the important elements and compounds are known experimentally, and third- and fourth-order constants are available for many of them, this scientific breakthrough may not seem to have much practical importance. But, from a broader perspective, it may.

The elastic properties of a material do not just determine its response to small strains. They are also the scaling parameters that measure the first-order differences in the strengths of materials. The classic models of the Peierls–Nabarro stress (or, perhaps more appropriately, the double-kink nucleation stress) that govern the onset of plasticity, the dislocation–obstacle interactions that produce hardening, and the shear and tensile instabilities that set the upper bounds on mechanical strength all scale linearly with the appropriate elastic

constants [2,3]. This scaling is borne out experimentally. For example, Fig. 1 plots typical hardness values of the common elements and compounds against the polycrystalline shear modulus. While the data divide according to bond type, and scatter appreciably, they support the classical idea that the elastic modulus is a first-order determinant of strength. It follows that a deep understanding of elastic behavior should enhance both the science and the practical control of mechanical strength.

As part of a study of the limits of strength in homogeneous deformation, we have recently completed *ab initio* calculations of the response of Al and Cu to homogeneous shear [4]. The calculations carry that shear to the point of instability, or the “ideal shear strength”. In the present paper, we shall briefly review those results, then discuss the similarities and differences in the large-strain elastic behavior of Al and Cu. In the fully relaxed case, the two have very similar strengths (when these are expressed in dimensionless form), but very different relaxation strains.

2. Method of calculation

The total energies of Al and Cu were computed as functions of strain using the pseudopotential total-en-

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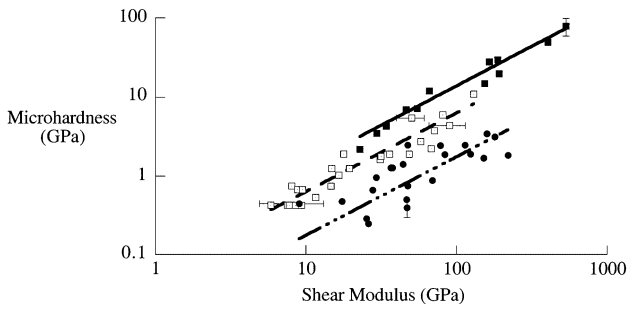


Fig. 1. Log-log plot of bulk hardness as a function of shear modulus. Solid line, solid squares refer to covalent compounds, dashed line, dotted squares refer to ionic compounds, solid circles, broken line refer to metals and alloys.

ergy scheme [5,6]. Computational details are given in Ref. [4]. The shear stress is found by straining the crystal in a series of incremental simple shears, calculating the energy and volume as functions of the strain, and taking the derivative of the energy with respect to the strain. The ideal shear strength (in the low-temperature limit) is the maximum value of this stress. In both Al and Cu, the shear strength is minimum for shear on the (1 1 1) plane in the $[1\ 1\ \bar{2}]$ direction. It is, therefore, useful to refer the displacements to a Cartesian coordinate system with a unit vector, \mathbf{e}_3 , perpendicular to the (1 1 1) plane and unit vectors \mathbf{e}_1 and \mathbf{e}_2 parallel to the $[1\ 1\ \bar{2}]$ and $[1\ \bar{1}\ 0]$ directions, respectively (Fig. 2). With this notation, an incremental simple shear in the $[1\ 1\ \bar{2}]$ direction on (1 1 1) takes the form,

$$\delta\epsilon = \epsilon_{13}(\mathbf{e}_1\mathbf{e}_3 + \mathbf{e}_3\mathbf{e}_1). \quad (1)$$

To increment the strain under fully relaxed conditions, we impose ϵ_{13} ($=\epsilon_{31}$), and adjust the other components of the strain tensor until their associated stresses vanish (specifically, until the calculated Hellman–Feynman stresses are <0.05 GPa). Since $\epsilon_{12} = \epsilon_{23} = 0$ by symmetry, the relaxation strains are stretches along the coordinate axes.

While there is no unique definition of finite strain [7], the three lattice parameters, \mathbf{a}^z , are defined at each step of the deformation and can be described by the three functions, $\mathbf{a}^z(n)$, where n is the number of incremental strain steps in the simulation. If $\mathbf{D}(n,m)$ is the Cartesian tensor that describes the deformation between steps m and n ,

$$\mathbf{a}^z(n) = \mathbf{a}^z(m) + \mathbf{D}_{ij}(n,m) \mathbf{a}_j^z(m). \quad (2)$$

Given $\mathbf{D}(n,m)$, the true strain, ϵ , and the engineering strain, ϵ^E , are defined as,

$$\epsilon_{ij}(n) = \frac{1}{2} \sum_{m=2}^n [\mathbf{D}_{ij}(m,m-1) + \mathbf{D}_{ji}(m,m-1)], \quad (3)$$

$$\epsilon_{ij}^E(n) = \frac{1}{2} [\mathbf{D}_{ij}(n,0) + \mathbf{D}_{ji}(n,0)]. \quad (4)$$

The derivatives of the energy with respect to the true

strain define the stresses that drive incremental deformation, and, therefore, the true strain is used to calculate the stress.

The energy is a unique function of the strain, ϵ_{13} , when either: (1) the crystal is unrelaxed, so ϵ_{13} is the only non-zero strain, or (2) the crystal is fully relaxed, so setting the value of ϵ_{13} fixes all the other strains. In either case, the conjugate shear stress is,

$$\tau = \sigma_{13} = \frac{1}{V} \frac{\partial E}{\partial \epsilon_{13}} = \frac{1}{V} \frac{\partial E}{\partial \gamma_{13}}, \quad (5)$$

where $\gamma_{ij} = \epsilon_{ij} + \epsilon_{ji} = 2\epsilon_{ij}$ is the shear, and V is the atomic volume at the applied strain. The relevant shear modulus, G' , is determined by the second-derivative, $\partial^2 E / \partial \gamma^2$. For shear in the $[1\ 1\ \bar{2}]$ direction on the (1 1 1) plane of fcc, the shear moduli are,

$$G'_u = C'_{55} = \frac{1}{3} [C_{11} + C_{44} - C_{12}], \quad (6)$$

$$G'_r = \frac{1}{S'_{55}} = \frac{3C_{44}(C_{11} - C_{12})}{4C_{44} + C_{11} - C_{12}}, \quad (7)$$

where G'_u governs the unrelaxed case, $\epsilon_{ij} = 0$ unless $ij = 13$ or 31 ($= 5$ in the Voigt notation), G'_r governs the relaxed case, $\sigma_{ij} = 0$ unless $ij = 13$ or 31 , the C_{ij} are the Voigt elastic constants for the cubic crystal, and C' and S' are, respectively, the Voigt elastic constants and compliances in the coordinate system shown in Fig. 2. The moduli govern incremental displacements from the current state and are, hence, functions of the strain.

3. Results

The results of the calculations are summarized in Tables 1–3 (reproduced from Ref. [4]) and in Fig. 3. Table 1 compares the calculated and experimental values for the lattice constants and shear moduli at zero applied strain. The close agreement indicates the accuracy of the calculations.

Fig. 3 plots the stress–strain relations of Al and Cu for relaxed shear. For comparison, we have included the sinusoidal curve for Cu suggested by Frenkel [8]. The stresses and strains at instability are tabulated in Tables 2 and 3. The results show the importance of elastic relaxation, which decreases the shear strength some 40% from the unrelaxed value. Interestingly, the normalized shear strengths of Al and Cu in the fully relaxed state are essentially identical ($0.085G'_r$) and are much closer to the classic Frenkel estimate ($0.1G$) than to the more modern estimates that have been preferred in recent years [3].

The elastic strain at shear instability is tabulated in Table 3. The imposed shear is γ_{13} , a displacement of the (1 1 1) planes in the $[1\ 1\ \bar{2}]$ direction. The relaxation

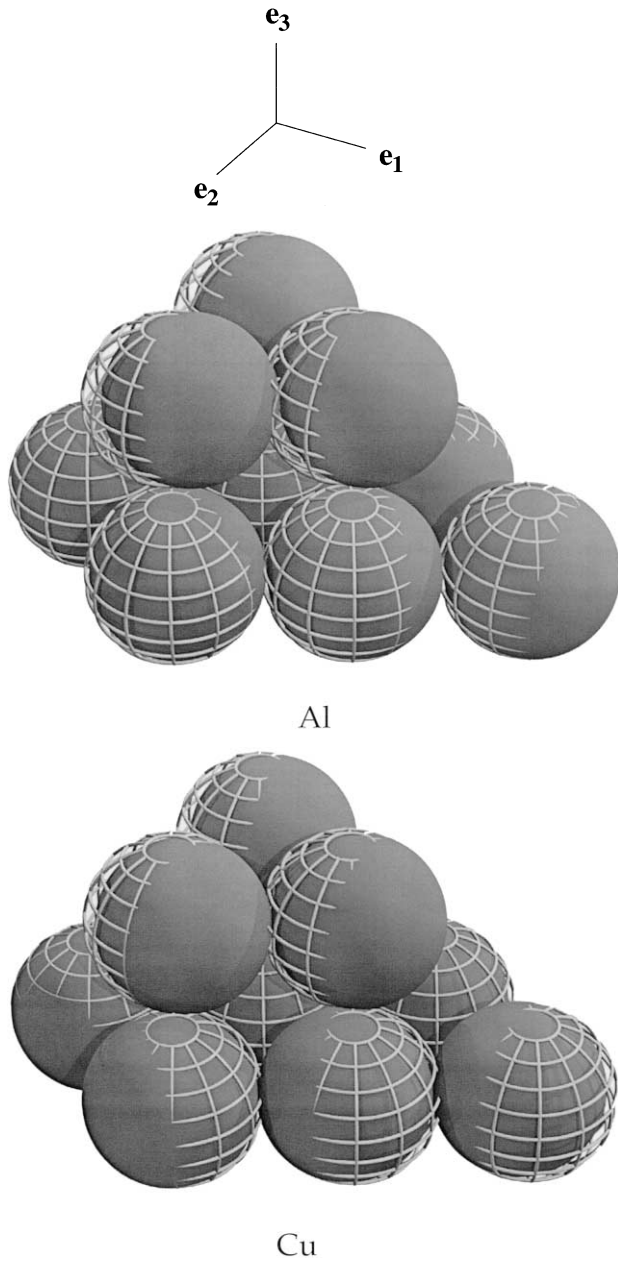


Fig. 2. Illustration of the atomic arrangement before and after unrelaxed shear in Al and Cu. The cages give the original atom positions in the fcc lattice, the solid spheres show atom positions at the point of shear instability. The Cartesian coordinate system is illustrated at left: $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} = \{[1\ 1\ \bar{2}], [1\ \bar{1}\ 0], [1\ 1\ 1]\}$.

strains are the stretches, ε_{11} and ε_{22} in the $(1\ 1\ 1)$ plane, and ε_{33} perpendicular to it. The primary shear strain (γ_{13}^E) at instability is nearly the same for Al and Cu (Table 3), and is significantly below the value (17.8%) that a rigid-ball model would produce.

However, the relaxation strains in the two cases are dramatically different (Fig. 2). Cu is relaxed by a shear in the $(1\ 1\ 1)$ plane in which a contraction in the direction of shear displacement (ε_{11}) is balanced by a perpendicular expansion (ε_{22}). The separation between $(1\ 1\ 1)$ planes is almost unchanged (ε_{33} small), so the

volume is almost constant. Al, on the other hand, is relaxed primarily by a shear in the $(1\ 1\ \bar{2})$ plane, with $\varepsilon_{33} \cong -\varepsilon_{22} > \varepsilon_{11}$. The $(1\ 1\ 1)$ interplanar spacing increases by $\approx 3\%$, and the volume increases by 1.4%.

4. Discussion

Both the similarities and differences in the behavior of Al and Cu merit discussion. The most striking similarities are the crystallography of the shear that produces minimum strength (the weak direction in both Al and Cu is in the $\langle 1\ 1\ 2 \rangle$ direction in a $\{1\ 1\ 1\}$ plane) and the virtual identity of the normalized shear strengths. The most striking dissimilarity is the qualitative difference in the relaxation strain.

The soft direction in shear: A shear in a $\langle 1\ 1\ 2 \rangle$ direction in a $\{1\ 1\ 1\}$ plane in a material with the fcc crystal structure is a shear that is associated with twinning in $\{1\ 1\ 1\}$ and with the partial slip at the

Table 1

Calculated and experimental lattice parameters and elastic moduli

	Al	Cu		
	Calculated	Experimenta l	Calculated	Experimenta l
Lattice constant (Å) ^a	4.12	4.05	3.57	3.61
(G _r ') (GPa) ^b	22 ± 3	24.5	30 ± 4	30.5
(G _u ') (GPa) ^b	27 ± 3	24.8	40 ± 4	40.8

^a Experimental values from Wyckoff [9].

^b Shear moduli are defined by Eqs. (6) and (7). Experimental Voigt elastic constants are from Nelson [10].

Table 2

Ideal shear strengths with and without structural relaxations

	Failure stress			
	τ_r (GPa)	τ_r/G'_r	τ_u (GPa)	τ_u/G'_u
Al	1.85 ± 0.1	0.084	3.4 ± 0.1	0.13
Cu	2.65 ± 0.2	0.088	4.0 ± 0.1	0.10

Table 3

Engineering strains at shear instability

	Failure strain (%)				
	γ_{13}^E	ε_{11}^E	ε_{22}^E	ε_{33}^E	$\Delta V/V_0$
Al	14.5	1	-3	3	1.4
Cu	13	-3	3	0.2	0.4

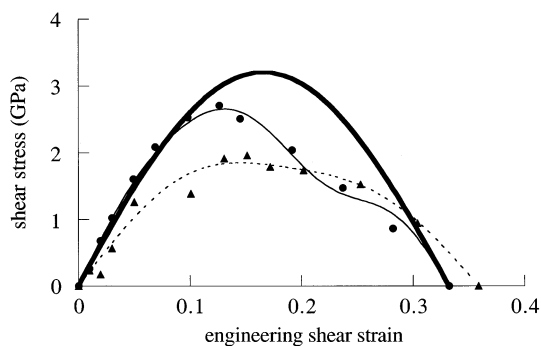


Fig. 3. Stress vs. engineering strain for Cu (solid circles and light solid line) and Al (solid triangles and dashed line). The heavy solid line is the stress predicted by a Frenkel sinusoidal model for Cu. The data points are the Hellman–Feynman stresses and the lighter weight lines represent the derivatives of the smoothed fits to the energies.

boundary of a stacking fault in $\{111\}$. Hence one would expect this shear to be the soft shear in materials like Cu that twin and form stacking faults. However, Al has a high stacking fault energy, and one might expect some other shear to be preferred. The reason that $\langle 112 \rangle \{111\}$ is the soft shear in Al can be explained by the fact that the applied shear is uniform and the local atomic coordination near the instability resembles that of the relaxed crystal more than that of a twinned or faulted one.

$$S_{\text{Al}}(\varepsilon = 0) = \begin{bmatrix} 0.0139 & -0.0051 & -0.0045 & 0 & -0.0019 & 0 \\ -0.0051 & 0.0139 & -0.0045 & 0 & 0.0019 & 0 \\ -0.0045 & -0.0045 & 0.0132 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.0408 & 0 & 0.0038 \\ -0.0019 & 0.0019 & 0 & 0 & 0.0408 & 0 \\ 0 & 0 & 0 & 0.0038 & 0 & 0.0380 \end{bmatrix} \text{ GPa}^{-1}, \quad (8a)$$

$$S'_{\text{Cu}}(\varepsilon = 0) = \begin{bmatrix} 0.0077 & -0.0038 & -0.0014 & 0 & -0.0069 & 0 \\ -0.0038 & 0.0077 & -0.0014 & 0 & 0.0069 & 0 \\ -0.0014 & -0.0014 & 0.0052 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.0328 & 0 & 0.0138 \\ -0.0069 & 0.0069 & 0 & 0 & 0.0328 & 0 \\ 0 & 0 & 0 & 0.0138 & 0 & 0.0230 \end{bmatrix} \text{ GPa}^{-1}. \quad (8b)$$

If bulk Al were strained beyond its shear instability, the instability would necessarily resolve itself in a shower of dislocations, twins or faults, whichever were easier to achieve. It is at this point that the choice between total dislocations, partial dislocations or twins would be made. Since even a small shear carries elastic energy equivalent to that of a high density of dislocations, the elastic energy of a crystal strained to instability is sufficient to carry it into whatever defect state is preferred.

The normalized shear strength: The close similarity between the normalized shear strengths of Al and Cu is probably fortuitous. The unrelaxed shear strengths are not that close ($\approx 0.13G'_u$ for Al vs. $\approx 0.1G'_u$ for Cu) and the relaxation patterns are very different. Nonetheless, since our recently published calculations for W also produce a shear strength near $0.085G'_r$, this appears to be a common value for the ideal shear strength of a metal [11].

The relaxation strain: While more detailed calculations will be conducted in the near future, the difference in the relaxation strains of Al and Cu can be explained, qualitatively, from their elastic behavior. To phrase this discussion, we first present the Voigt compliance tensors (Eqs. (8a) and (8b)) for Al and Cu in the form they take after transformation into the coordinate system shown in Fig. 2.

Since the $[111]$ direction is a three-fold symmetry axis in fcc, the compliance tensor has a superficially trigonal symmetry; the non-diagonal elements S'_{15} and S'_{25} do not ordinarily vanish. However, $S'_{15} = -S'_{25}$ and, since $S'_{35} = 0$, the imposition of a shear stress in the $[11\bar{2}]$ direction on (111) , which is τ_{13} (or τ_5 in the Voigt notation) produces a shear of type $[11\bar{2}](111)$ that is relaxed by a shear in the (111) plane, $\varepsilon_{11} = -\varepsilon_{22}$, of precisely the type that is dominant in Cu (Table 3).

However, the value of S'_{15} is determined by the elastic anisotropy factor, A ($= C_{11} - C_{12} - 2C_{44}$), according to the relation,

$$S'_{15} = \frac{\Delta}{3\sqrt{2}(C_{11} - C_{12})C_{44}}. \quad (9)$$

It follows that S'_{15} increases with A , and vanishes when $A = 0$. The strong elastic anisotropy of Cu has the consequence that its elastic, in-plane relaxation is much greater than that in the more isotropic Al.

$$S_{\text{Al}}(\varepsilon = 0.15) = \begin{bmatrix} 0.0135 & -0.0055 & -0.0027 & 0 & 0.0026 & 0 \\ -0.0055 & 0.0154 & -0.0072 & 0 & -0.0063 & 0 \\ -0.0027 & -0.0072 & 0.0176 & 0 & 0.0177 & 0 \\ 0 & 0 & 0 & 0.0353 & 0 & 0.0092 \\ 0.0026 & -0.0063 & 0.0177 & 0 & 0.0730 & 0 \\ 0 & 0 & 0 & 0.0092 & 0 & 0.0394 \end{bmatrix} \text{ GPa}^{-1}, \quad (10a)$$

$$S_{\text{Cu}}(\varepsilon = 0.13) = \begin{bmatrix} 0.0087 & -0.0046 & -0.0027 & 0 & -0.0128 & 0 \\ -0.0046 & 0.0083 & -0.0004 & 0 & 0.0109 & 0 \\ -0.0027 & -0.0004 & 0.0067 & 0 & 0.0097 & 0 \\ 0 & 0 & 0 & 0.0239 & 0 & 0.0109 \\ -0.0128 & 0.0109 & 0.0097 & 0 & 0.0680 & 0 \\ 0 & 0 & 0 & 0.0109 & 0 & 0.0217 \end{bmatrix} \text{ GPa}^{-1}. \quad (10b)$$

A shear of type $[1\ 1\ \bar{2}](1\ 1\ 1)$ breaks the symmetry of the fcc crystal. The symmetry of the strained crystal allows $S'_{15} \neq -S'_{25}$ and $S'_{35} \neq 0$, so there can be a relaxation strain, ε_{33} , perpendicular to the $(1\ 1\ 1)$ plane and a net volume change. The symmetry change is exploited very quickly in the almost isotropic Al crystal, which rapidly develops significant values of ε_{33} , $\varepsilon_{11} + \varepsilon_{22}$, and ΔV . In the anisotropic Cu crystal, in contrast, the finite-strain effect is small, and the relaxation strain is only slightly perturbed from its symmetry in the relaxed state.

The qualitative difference between the relaxation strains of Al and Cu is also observed experimentally. Approximate compliance tensors of Al and Cu at the shear instability are presented above (Eqs. (10a) and (10b)), as estimated from the third-order elastic constants tabulated in [10]. Even though the experimental data were taken at strains of only a fraction of a percent, the measured third order elastic constants do predict that the S'_{15} and S'_{25} compliances of Al will change sign. The compliances also predict the relative magnitudes and sign of the relaxations in Al, and the signs of the relaxations in Cu. Finally, one can extract estimates of the sign and magnitude of the volume change with applied shear by summing S'_{15} , S'_{25} and S'_{35} . For Al, the volumetric compliance is 1.4% and for Cu, 0.8%. These figures are again qualitatively consistent with the theoretical results given in Table 3.

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